

**Next Generation System
Modeling of NTR Systems**

John J. Buksa and William J. Rider
Los Alamos National Laboratory
October 22, 1992

Los Alamos

Introduction

- ☐ NTR Modeling Challenges
- ☐ Current Approaches
- ☐ Shortcomings of Current Analysis Methods
- ☐ Future Needs
- ☐ Present Steps Toward These Goals

Los Alamos

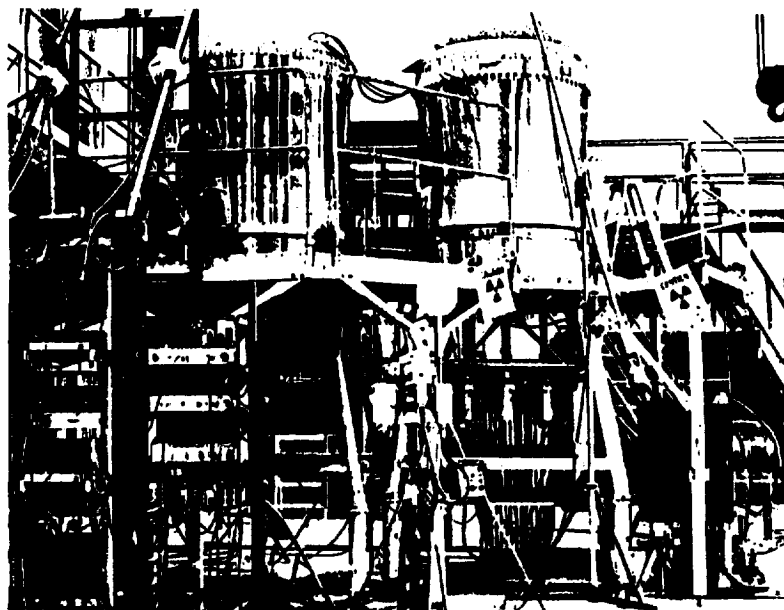
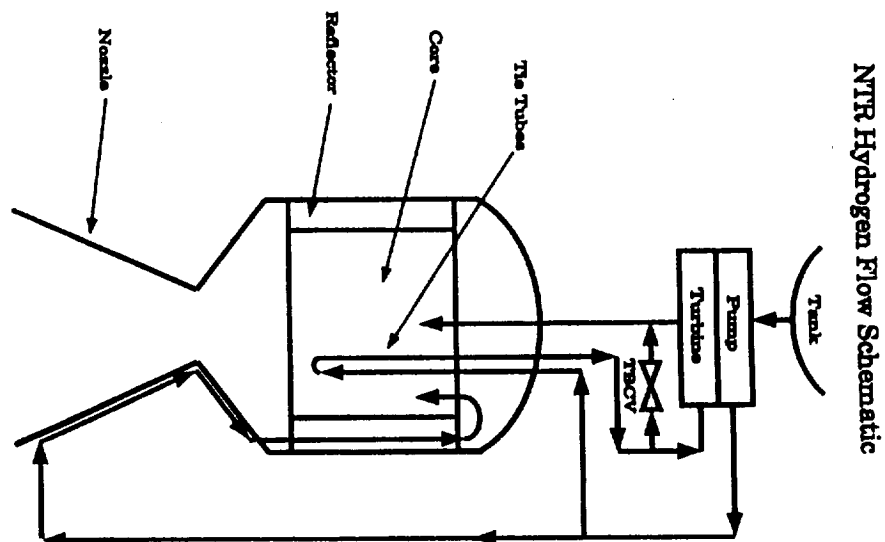
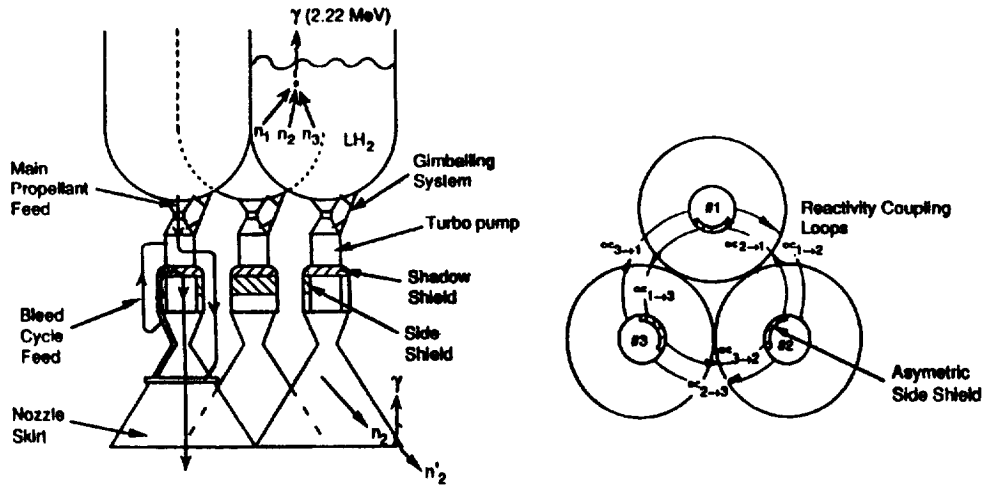


Figure 1. The Coupled Cores in Kiva-3, Pajarito Site. "Test Kiwi" is on the left, and PARKA is on the right.

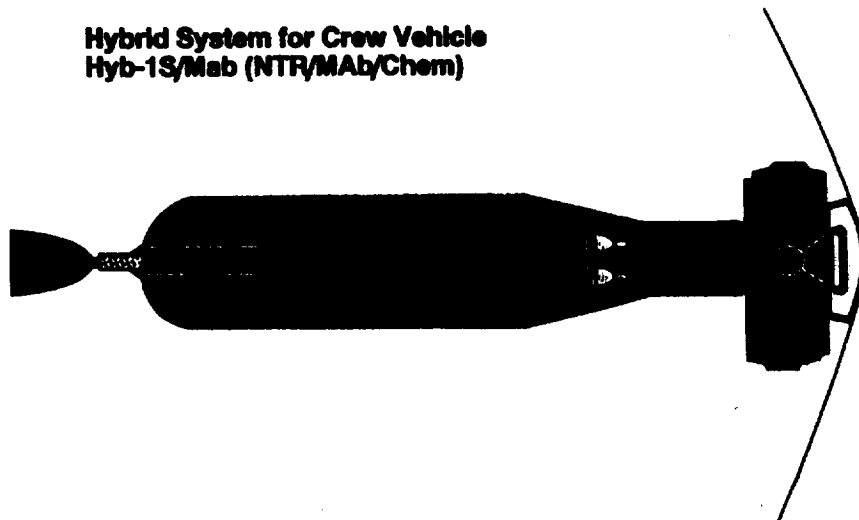
ENGINE COUPLING PHENOMENA

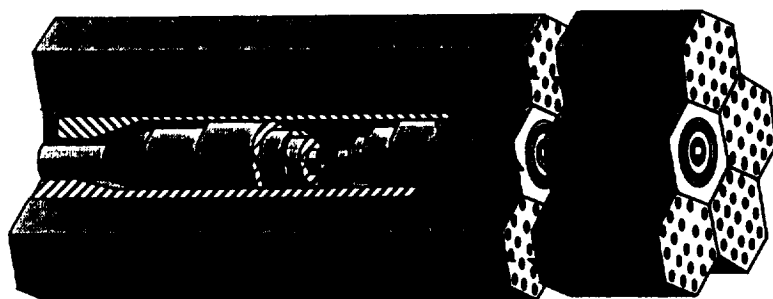
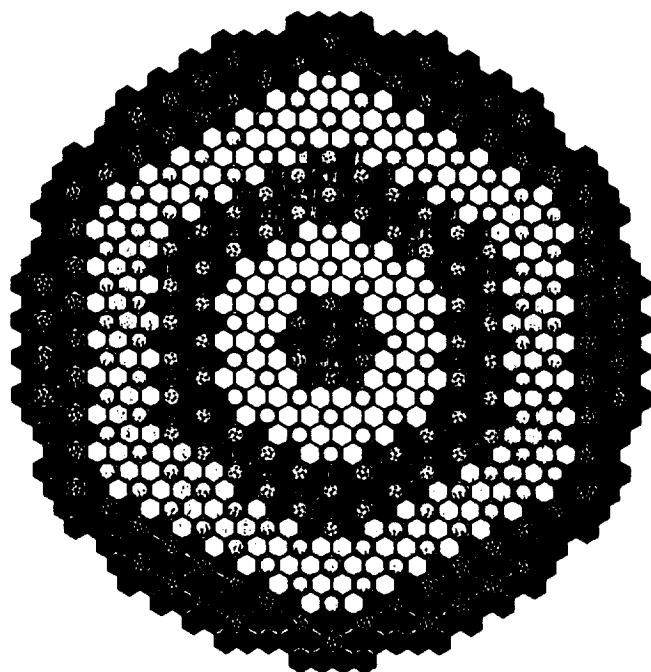


3/82

Los Alamos

**Hybrid System for Crew Vehicle
Hyb-1S/Mab (NTR/MAB/Chem)**



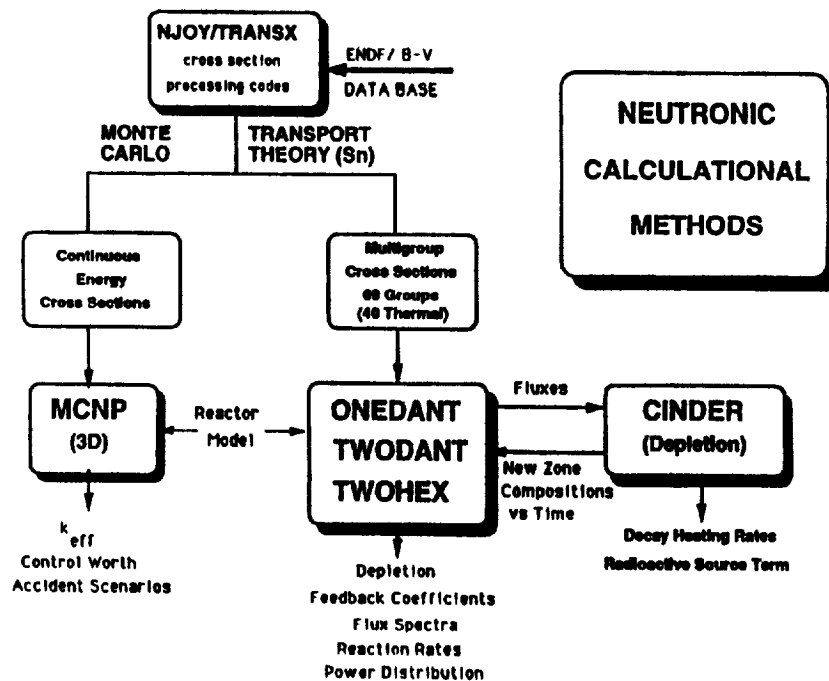


3D NTR Cluster

Introduction: Modeling Applications

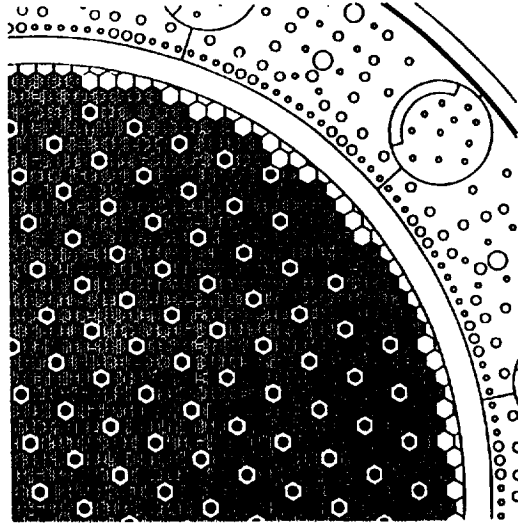
- Design: performance (SS operation) and lifetime (fuel / criticality)
- Startup and Shutdown
(two phase T-H, neutronics, kinetics, heat transfer, low strain rate hydro)
- Water Immersion
(kinetics, neutronics, all hydro)
- Impaction
(kinetics, neutronics, high strain rate hydro)
- Engine-Out Operations
(all except high strain rate hydro)

Los Alamos



Los Alamos

DETAILED MCNP MODELING OF NUCLEAR THERMAL ROCKETS – WESTINGHOUSE NRX-A6 REACTOR



3/92

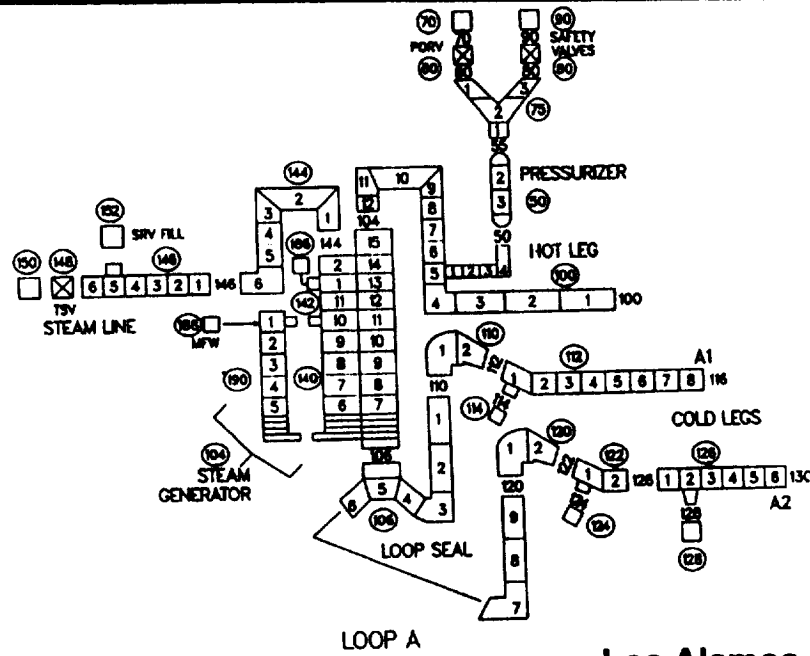
Los Alamos

Thermal-Hydraulic Analysis Methods

- Extensive experience in both space and terrestrial reactors
- **TRAC**
 - Developed for LOCA analysis of PWRs
 - Highly developed models for two-phase flow
 - Low/zero gravity models are available
 - Useful for facility/more general system analysis
- **HERA**
 - Developed for solid core terrestrial reactors
 - Useful for the thermal analysis of general systems including space nuclear systems
- **KLAXON**
 - New thermal hydraulic systems code designed specifically for gas cooled, space reactors
- **THROHPUT**
 - State-of-the-art heat pipe modeling from startup to shutdown

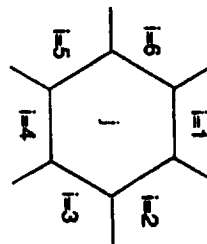
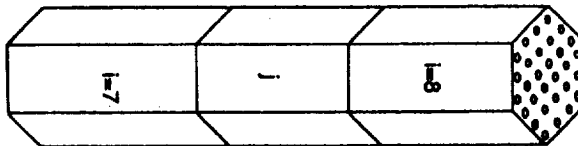
Los Alamos

Example TRAC Noding Diagram



Los Alamos

Description of HERA



- Helium Reactor Analysis
- Fully three-dimensional allowing for complex geometries to be accurately represented.
- Flexible input allows a large number of test cases.
- The code computes solution with minimal computational effort.

4

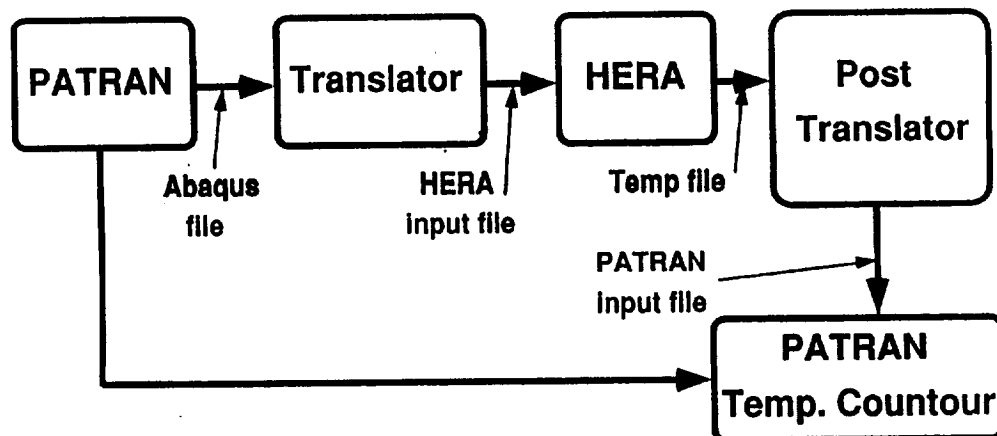
Thermal-Hydraulic Modeling: Prismatic Fuel

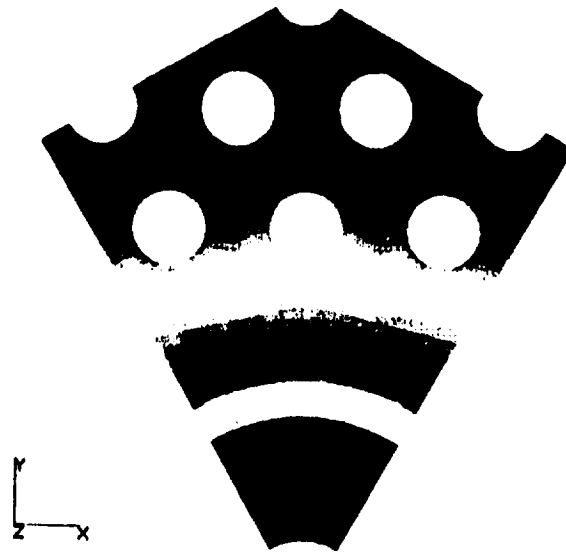
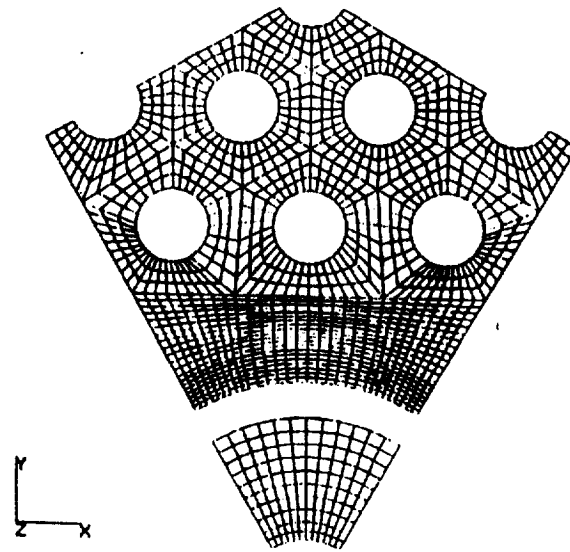
- HERA: HEllium/Hydrogen Reactor Analysis
- Used to model reactor core and core components with axially homogeneous construction
- Three-dimensional, fully transient, arbitrary user defined geometries
- Programmed to be computationally efficient, especially on vector supercomputers
- Currently exists in stand-alone mode and coupled to TRAC. Connection to KLAXON is planned
- PATRAN grid generator and visualization translators currently being written
- Coupling to Storm's corrosion model envisioned → **Core Lifetime**
- Component and core T-H model planned (fuel element, support element, and periphery)

Los Alamos

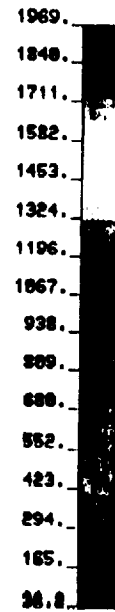
Methodology: New

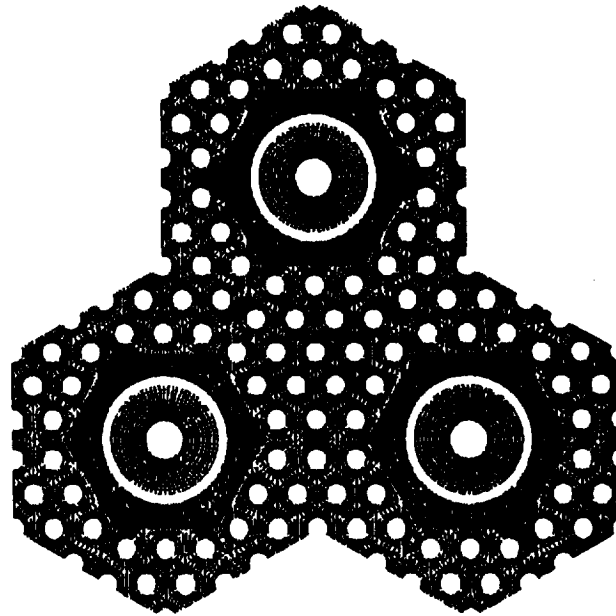
Specific Outline:



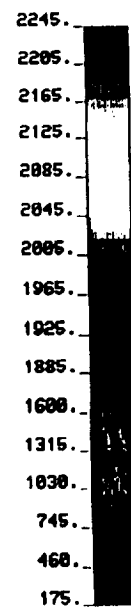


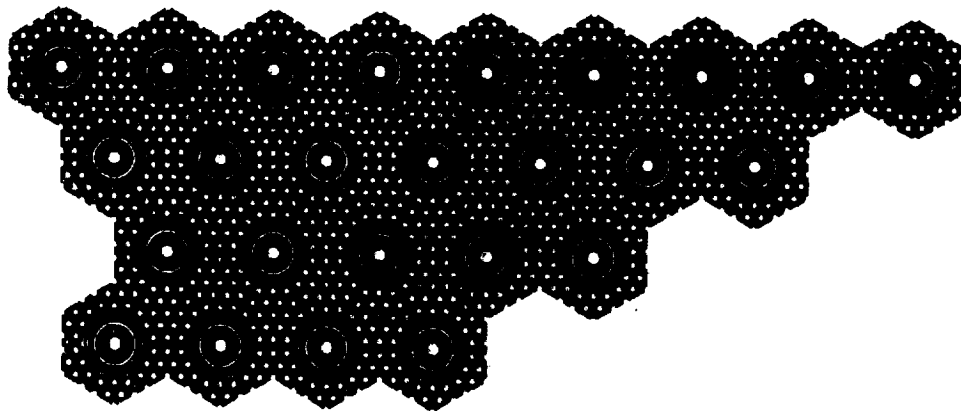
TEMPERATURE CONTOUR
 SECTION
 FIRE FISHING





TEMPERATURE CONTOUR
TIE ROD AND FUEL ELEMENT CLUSTER
FINE MESHING



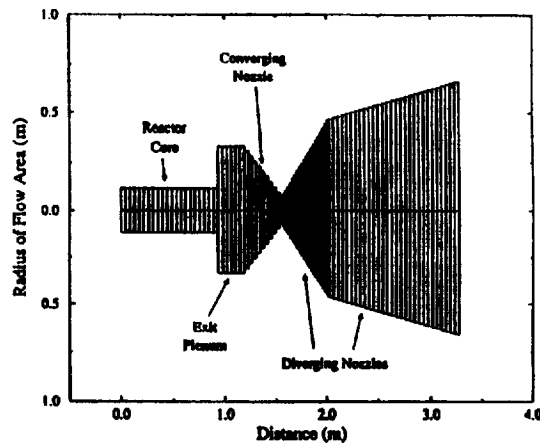


KLAXON GAS-COOLED REACTOR SYSTEMS MODELING CODE

Time-dependent analysis of systems operating with compressible gas working fluids. TRAC-like pipe, plenum, etc. component models, fill and break capabilities, and advanced flow modeling numerics for shock following in nozzles.

Future Development

- Connection to HERA
- Validation with systems data



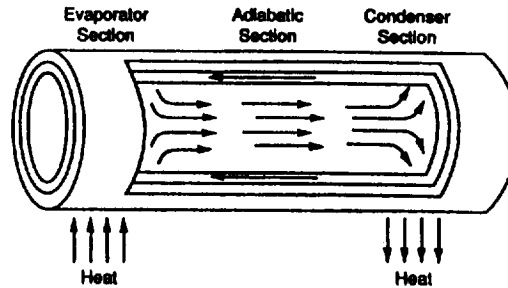
NTR Geometry

Los Alamos

THROHPUT HEAT PIPE MODELING CODE

Transient thermal-hydraulic heat pipe modeling code with:

- Multi-region capability (wall, fluid, mixed, gas)
- 2-D convection and conduction heat transfer
- Li melt model
- Gravity and non-gravity capillary pressure models



Future development:
Benchmarking and validation
with LANL experiments

Heat Pipe Operation

3/92

Los Alamos

Los Alamos
Los Alamos National Laboratory
Los Alamos, New Mexico 87545

Why Level 3/4 Model Development?

- Level 3/4 Improvements
 - Integral versus Ad hoc
 - Physics versus Assumptions
 - Confidence versus Safety Margin
 - Machine versus Human Intervention
- Examples
 - Reactor Compaction/Immersion Accidents
 - Reactor Startup

1

Future Needs

- ☐ **Better All Around Resolution of Problems**
- ☐ **System Design Optimization Tools**
- ☐ **Complete Utilization of Modern Technology
(Computers and Algorithms)**
- ☐ **Use of Integrated Physics Codes**

Los Alamos

LOS ALAMOS
LOS ALAMOS NATIONAL LABORATORY

**REACTOR DESIGN AND
ANALYSIS GROUP**

Los Alamos Perspective

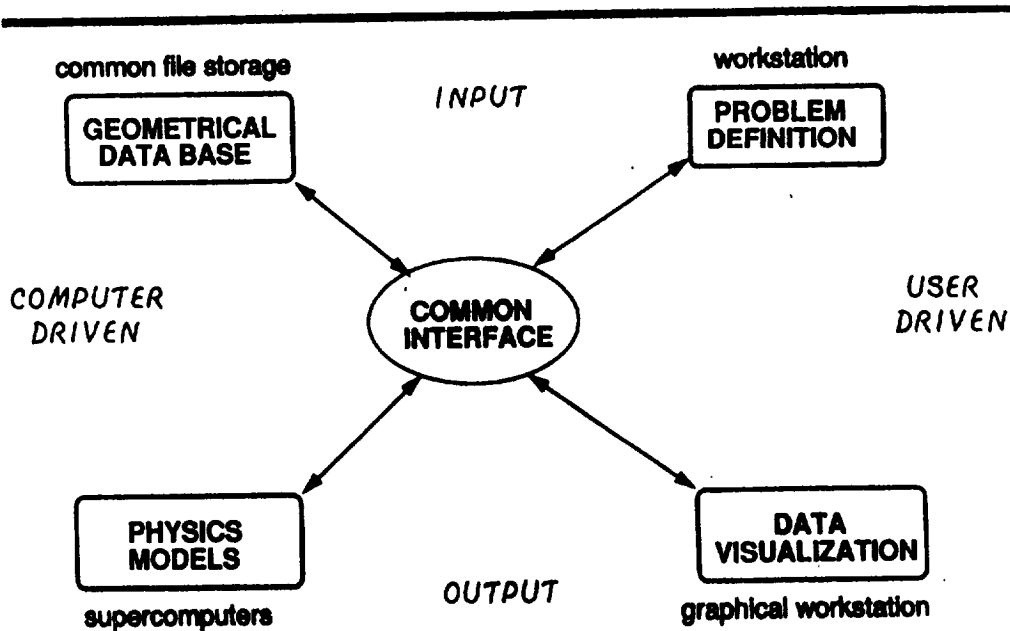
- **Emphasis on Simulation Instead of Testing**
 - current ES&H environment dictates reduced testing of nuclear systems
- **Interagency NTP Modeling Team**
 - Role, Impact, Importance, Visibility
- **Effort Should be Commensurate With the SEI**
 - ambitious, high profile, high tech, national importance

The Need for New Code Development in Level 3/4

- No "Real" Level 3/4 Codes Exist
- Codes will be Heavily Relied on
- Testing will be Restricted by ES&H Requirements
- Current Codes are Designed to Analyze Primarily Terrestrial Reactors
- Current Codes use Outdated Methodologies
- Current Codes are Designed for Older Computer Architectures

2

Advanced Architecture: Description



Los Alamos

- Neutronics (including cross-sections, dosimetry)
- Spatial Kinetics
- Generation/Depletion
- Thermal-Hydraulics (two phase)
- Low Strain Rate Hydro
- High Strain Rate Hydro (solid and fluid)
- Heat transfer (conduction, radiation)
- Chemistry/Materials

Los Alamos

Los Alamos
Los Alamos National Laboratory
Los Alamos, New Mexico 87545

LANL Current Status

- Outlined Needs and Requirement for Level 3/4 Code Development
- Investigated LANL Capability
- Example LANL Capability
 - NIKE — A time-dependent S_n radiation transport code with arbitrary 3-D meshes on a CM (or Cray)
 - NIKE is coupled to PAGOSA/X3D for high strain rate hydrodynamics on CM (or Cray)
 - Genesis of Level 3/4 code capability for convection/immersion accident analysis
 - Starting demonstrative NIKE/PAGOSA NTR analysis effort
 - Thermal-hydraulic work continues with work on improving both KLAXON and HERA

Other Laboratory Capability

- Fluid dynamics codes
 - Developed for a large range of physical situations varying from incompressible to highly compressible flows
 - Advanced methodologies
- High Strain Rate Solid/Hydrodynamics
 - Applicable to events involving reactor impaction/disassembly
 - Examples: launch accidents, reentry, water immersion
 - Coupled directly to other physical phenomena (neutronics for instance)
 - Advanced methodologies
- High Performance Computing
 - One of two DOE centers of excellence
 - ICN (3 CMs, 7 Cray YMPs)
 - ACL

Los Alamos

ADVANCED COMPUTING LABORATORY

Acting as a university/industrial/laboratory interface for state of the art computations, emphasizing:

- State of the art hardware for massively parallel computation (largest CM-2s and CM-5 in the nation)
- Wide area gigabit network for distributed parallel computing (using ANSI standard: HIPPI)
- Advanced scientific visualization using high speed networking and parallel computational methods
- Software tools/algorithms development for distributed parallel computation (NSF Science & Tech. center: CRPC)
- Emphasizing "real" applications running in parallel environment (Grand Challenges and beyond)

Purposes of the ACL

- To respond to the rapid changes in hardware and software
- To investigate new "Grand Challenge" computing environments
- To provide more "access" to Los Alamos from the outside world
- Provide high performance testbed for networking and visualization
- Stimulate practical algorithm development for massively parallel computing
- Function as one of the Dept of Energy High Performance Computing Research Centers

Los Alamos

Table 1: TODAY

Project	Description	Operations	Memory	IO/Access
Porous Media	2-d immiscible flow	10^{16}	8 Gbytes	40 GBytes
Novel Materials	2-d molecular dynamics	10^{14}	500 Mbytes	64 GBytes
	3-d multimaterial hydro (200 ³ pts)	10^{15}	8 GBytes	100GBytes
Plasma physics	transport scaling	10^{15}	8 GBytes	200 GBytes
Global Ocean	decade, 20 levels, 1/2°	10^{15}	500 MBytes	250 GBytes
Brain Topology	3-d reconstruction	10^{13}	200 MBytes	10 GBytes
QCD	quenched lattice (32x32x32x64)	10^{16}	500 MBytes	500 MBytes

Table 1: TOMORROW

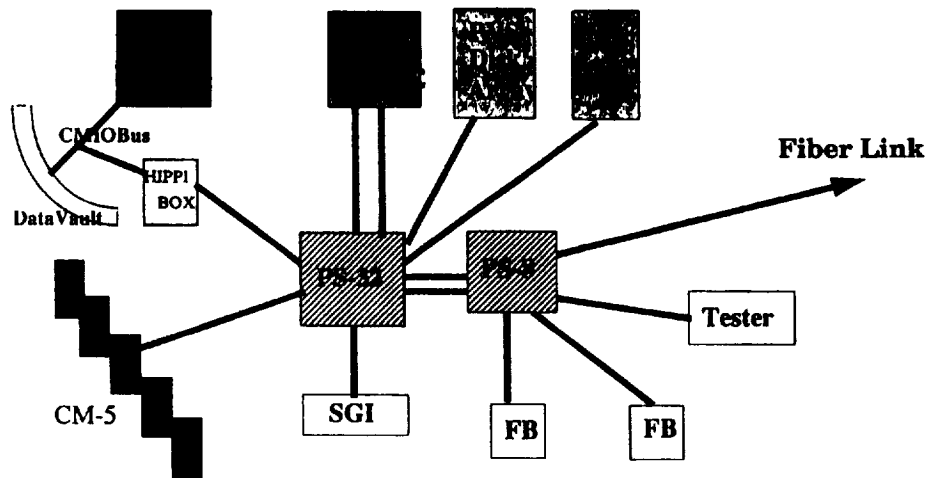
Porous Media	3-d immiscible flow	10^{18}	1 Tbytes	4 TBytes
Novel Materials	3-d molecular dynamics	10^{18}	20 Gbytes	3 TBytes
	3-d multimaterial hydro (1000^3 pts)	10^{18}	1 TBytes	20TBytes
Plasma physics	numerical Tokamak	10^{18}	1 TBytes	100 TBytes
Global Ocean	century, 40 levels, $1/4^\circ$	10^{17}	4 GBytes	20 TBytes
Brain Topology	3-d reconstruction	10^{15}	15 GBytes	1 TBytes
QCD	quenched lattice (64x64x64x128)	10^{18}	8 GBytes	8 TBytes

Los Alamos

Applications on the CM-2

- QCD
- Condensed Matter Physics
- Free Lagrange Hydrodynamics
- Global Ocean Model
- Lattice Gas (porous media)
- Oil Reservoir: Mobil (11Gflops sustained)
- Tokamak Fluid Turbulence
- Fokker Planck
- Crystal Formation
- Many Body Problem
- Plasma Particle Simulations
- Molecular Dynamics
- Neural Networks

Existing ACL HIPPI Network



Los Alamos

PAGOSA

-
- ☐ A 3-D Multi-Material Hydrodynamics Code on the Connection Machine
 - ☐ High-Speed Hydrodynamics and High-Rate Deformation of Solids
 - ☐ Eulerian, Second-Order Predictor Corrector Lagrangian Step with Third-Order High-Resolution Advection
 - ☐ High-Resolution Interface Reconstruction Algorithm
 - ☐ Highly Efficient for the Connection Machine

Los Alamos

The NIKE Codes

- NIKE-R
 - 3-D Rectangular Mesh
 - Corner Finite-Difference Scheme
- NIKE-T
 - 3-D Arbitrarily-Connected Tetrahedral Mesh
 - Linear-Continuous Finite-Element Discretization
- Common Characteristics
 - Solve Even-Parity S_n Transport Equation with Anisotropic Scattering in Cartesian Geometry
 - Time-Dependent, Steady-State, k or α Eigenvalue Calculations
 - Essentially Positive Solutions - No Flux Fixup
 - Inner and Outer Iteration DSA - Unconditionally Stable and Effective
 - Very Efficient Simplified P_n Option - No Ray Effects

Conclusions

- ☐ Current Modeling Approaches are Generally Inadequate
- ☐ In the Future Modeling will be Relled on Heavilly
- ☐ Los Alamos has begun to Lay the Groundwork for Future Modeling Capabillities